Statistical mechanics

- Large systems
- Finite temperature
- Grand canonical ensemble
- Statistical operator $\hat{\rho}_G = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z_G}$
- with $\beta = (k_B T)^{-1}$
- and μ chemical potential
- Grand partition function

$$Z_G = \mathrm{Tr}\left(e^{-\beta(\hat{H}-\mu\hat{N})}\right)$$

$$= \sum_N \sum_n \langle \Psi_n^N | e^{-\beta(\hat{H}-\mu\hat{N})} | \Psi_n^N \rangle = \sum_N \sum_n e^{-\beta(E_n^N - \mu N)}$$

Thermodynamic potential

- Standard result $\Omega(T, V, \mu) = -k_B T \ln Z_G$
- and therefore $\hat{\rho}_G = e^{\beta(\Omega - \hat{H} + \mu\hat{N})}$
- Ensemble averages $\langle \hat{O} \rangle = \mathrm{Tr}\,\left(\hat{\rho}_G \hat{O}\right) = \dfrac{\mathrm{Tr}\,\left(e^{-\beta(\hat{H}-\mu\hat{N})}\hat{O}\right)}{\mathrm{Tr}\,\left(e^{-\beta(\hat{H}-\mu\hat{N})}\right)}$
- Noninteracting systems replace $\hat{H} \rightarrow \hat{H}_0$
- Summing over complete sets of states in Fock space can also be accomplished by summing over all possible occupations of sp states in occupation number representation!
- Replace relevant operators by eigenvalues:

$$\hat{H}_0 \left| n_1 ... n_\infty \right\rangle = \sum_i n_i \varepsilon_i \left| n_1 ... n_\infty \right\rangle$$

$$\hat{N} \left| n_1 ... n_\infty \right\rangle = \sum_i n_i \left| n_1 ... n_\infty \right\rangle$$

- Apply

$$\begin{aligned}
Z_0 &= \sum_{n_1 ... n_\infty} \left\langle n_1 ... n_\infty \right| e^{-\beta(\hat{H}_0 - \mu\hat{N})} \left| n_1 ... n_\infty \right\rangle \\
&= \sum_{n_1 ... n_\infty} \left\langle n_1 ... n_\infty \right| e^{-\beta(\sum_i \varepsilon_i n_i - \mu \sum_i n_i)} \left| n_1 ... n_\infty \right\rangle \\
&= \sum_{n_1 ... n_\infty} \exp\left\{\beta(\mu n_1 - \varepsilon_1 n_1)\right\} ... \exp\left\{\beta(\mu n_\infty - \varepsilon_\infty n_\infty)\right\} \\
&= \prod_{i=1}^{\infty} \mathrm{Tr}\left(\exp\left\{-\beta(\varepsilon_i - \mu) n_i\right\}\right)
\end{aligned}$$

Noninteracting grand partition function

- Yields

$$Z_0 = \sum_{n_1 \ldots n_\infty} \exp\{\beta(\mu n_1 - \varepsilon_1 n_1)\} \ldots \exp\{\beta(\mu n_\infty - \varepsilon_\infty n_\infty)\}$$

$$= \prod_{i=1}^{\infty} \mathrm{Tr}\left(\exp\{-\beta(\varepsilon_i - \mu) n_i\}\right)$$

- with Tr including a summation over possible occupation numbers
- Bosons: all occupation numbers possible

$$Z_0^B = \prod_{i=1}^{\infty} \sum_{n=0}^{\infty} [\exp\{\beta(\mu - \varepsilon_i)\}]^n = \prod_{i=1}^{\infty} [1 - \exp\{\beta(\mu - \varepsilon_i)\}]^{-1}$$

- Thermodynamic potential

$$\Omega_0^B(T,V,\mu) = -k_B T \ln \prod_{i=1}^{\infty} [1 - \exp\{\beta(\mu - \varepsilon_i)\}]^{-1}$$

$$= k_B T \sum_{i=1}^{\infty} \ln[1 - \exp\{\beta(\mu - \varepsilon_i)\}]$$

- Average particle number

$$N = \langle N \rangle = -\left(\frac{\partial \Omega_0^B}{\partial \mu}\right)_{TV}$$

$$\langle N \rangle \equiv \sum_{i=1}^{\infty} n_i^0 = \sum_{i=1}^{\infty} \frac{1}{\exp\{\beta(\varepsilon_i - \mu)\} - 1}$$

Noninteracting fermions at finite T

- Restriction to 0 and 1 for occupation numbers

$$Z_0^F = \prod_{i=1}^{\infty} \sum_{n=0}^{1} \left[\exp\{\beta(\mu - \varepsilon_i)\}\right]^n = \prod_{i=1}^{\infty} \left[1 + \exp\{\beta(\mu - \varepsilon_i)\}\right]$$

- Thermodynamic potential

$$\Omega_0^F(T, V, \mu) = -k_B T \sum_{i=1}^{\infty} \ln\left[1 + \exp\{\beta(\mu - \varepsilon_i)\}\right]$$

- Particle number

$$\langle N \rangle \equiv \sum_{i=1}^{\infty} n_i^0 = \sum_{i=1}^{\infty} \frac{1}{\exp\{\beta(\varepsilon_i - \mu)\} + 1}$$

BEC in infinite systems

- Ground state of noninteracting bosons: all in lowest sp level
- This limit is approached when T $\rightarrow$ 0
- boson spectrum $\varepsilon(k) = \dfrac{\hbar^2 k^2}{2m}$
- As before $\sum_i \rightarrow \dfrac{\nu V}{(2\pi)^3} \int d\boldsymbol{k}$
- Transform to energy integral

$$\frac{\nu V}{(2\pi)^3}\, 4\pi k^2\, dk = \frac{\nu V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{\varepsilon d\varepsilon}{2\varepsilon^{1/2}} = \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2} d\varepsilon$$

- Thermodynamic potential

$$\begin{aligned} \Omega_0^B &= k_B T\, \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon\ \varepsilon^{1/2} \ln\left[1 - \exp\left\{\beta(\mu - \varepsilon)\right\}\right] \\ &= -\frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{2}{3} \int_0^\infty d\varepsilon\ \frac{\varepsilon^{3/2}}{\exp\left\{\beta(\varepsilon - \mu)\right\} - 1} \end{aligned}$$

BEC

- Energy $$E = \sum_i n_i^0 \varepsilon_i = \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \, \frac{\varepsilon^{3/2}}{\exp\{\beta(\varepsilon - \mu)\} - 1}$$
- Particle number $$N = \sum_i n_i^0 = \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \, \frac{\varepsilon^{1/2}}{\exp\{\beta(\varepsilon - \mu)\} - 1}$$
- Note $\Omega = -PV$ so one confirms ideal gas $PV = \frac{2}{3}E$
- Denominator represents occupation so may not become negative so chemical potential such that $\varepsilon - \mu \geq 0$ so here $\mu \leq 0$
- Fix density and lower temperature: $|\mu|$ should decrease
- The limit $\mu = 0$ for $$\begin{aligned} N &= \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \, \frac{\varepsilon^{1/2}}{\exp\{\varepsilon / k_B T_0\} - 1} \\ &= \frac{\nu V}{4\pi^2} \left(\frac{2m k_B T_0}{\hbar^2}\right)^{3/2} \int_0^\infty dx \, \frac{x^{1/2}}{\exp(x) - 1} \\ &= \frac{\nu V}{4\pi^2} \left(\frac{2m k_B T_0}{\hbar^2}\right)^{3/2} \zeta(\frac{3}{2}) \frac{1}{2}\sqrt{\pi} \end{aligned}$$

BEC

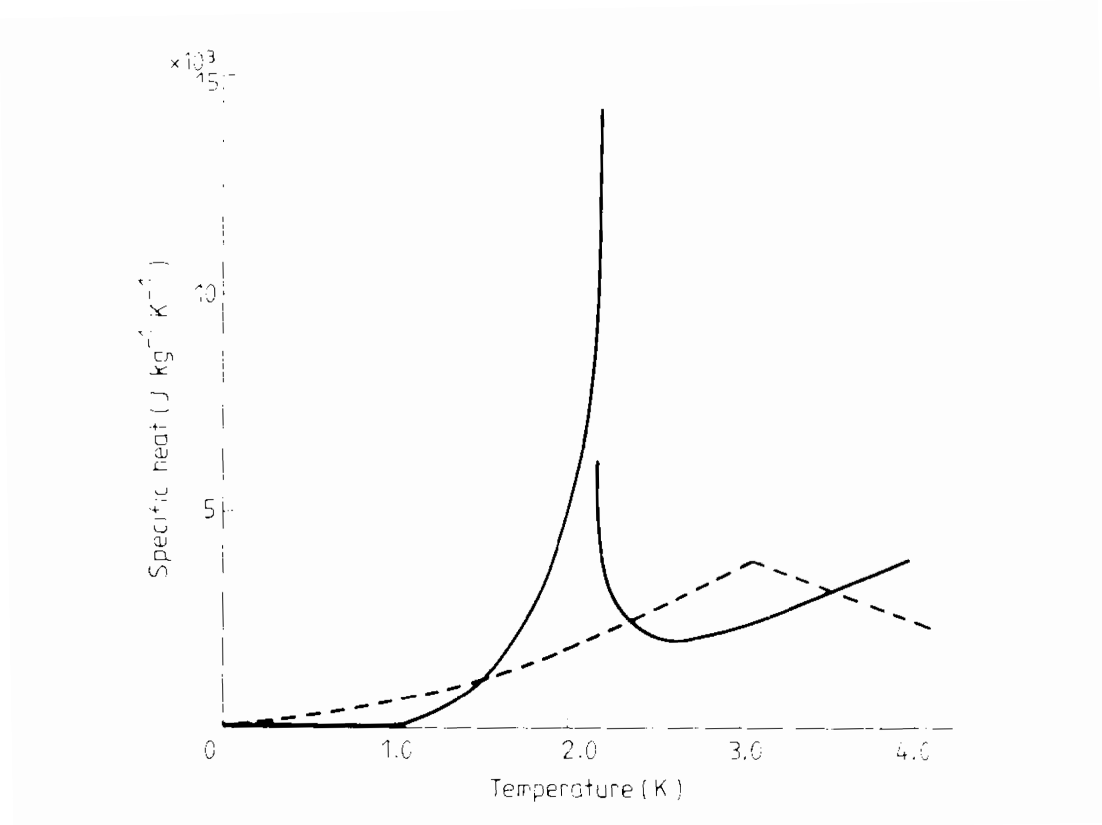
- Rewrite $$T_0 = \frac{3.31}{\nu^{2/3}} \frac{\hbar^2}{mk_B} \left(\frac{N}{V}\right)^{2/3}$$
- with $\zeta(\frac{3}{2}) = 2.612$ Riemann ζ-function
- For temperatures below T_0
  integral only yields particles with $\varepsilon > 0$
  so those particles represented by $N_{\varepsilon>0}(T) = N\left(\frac{T}{T_0}\right)^{3/2}$
- Remaining particles must all have $\varepsilon = 0$

$$N_{\varepsilon=0}(T) = N\left[1 - \left(\frac{T}{T_0}\right)^{3/2}\right]$$

- Macroscopic occupation (~N) of single state $\rightarrow$ BEC

BEC for ^{4}He

- Check that at T_0 there is a discontinuity in the slope of the specific heat (see Fetter and Walecka)
- For ^{4}He with $\rho = 0.145 \text{ g cm}^{-3}$ $\quad T_0 = 3.14 \text{ K}$
- Experimental transition at $T_0 = 2.2 \text{ K}$ and ...
- called λ transition
- $N_0 \sim 10\%$



Tilley & Tilley
Superfluidity & Superconductivity

- Superfluidity ≠ ideal gas but transition still related to BEC!?

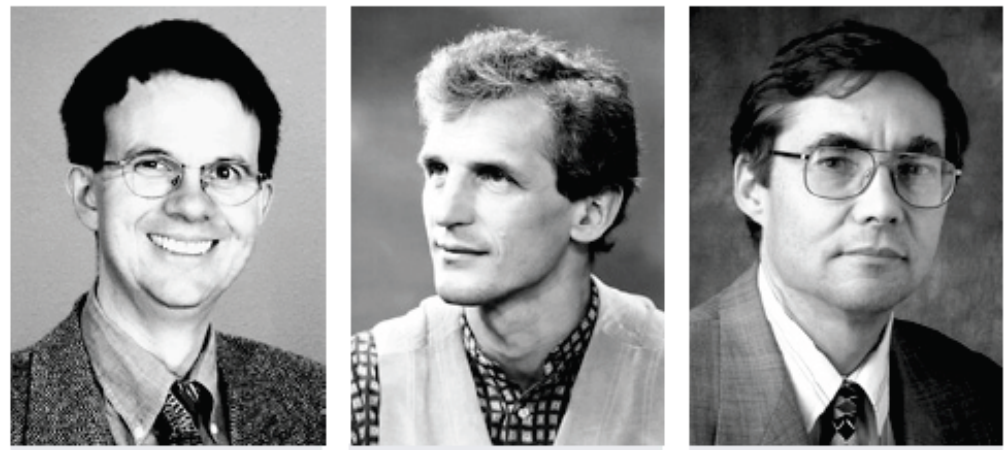
BEC in traps

- Laser cooling & magneto-optical trapping techniques
- Evaporative cooling
- Atomic gases are metastable
- Why?
- Temperatures $500 \text{ nK to } 2\mu\text{K}$
- Densities $\text{few } \times 10^{14} \text{atoms/cm}^3$
- Scales 10s to 100s of μm
- Magnetic traps for alkali atoms look like harmonic oscillators with different oscillator lengths

$$V_{ext}(\boldsymbol{r}) = \frac{1}{2} m \left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right)$$

The Nobel Prize in Physics 2001

"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"



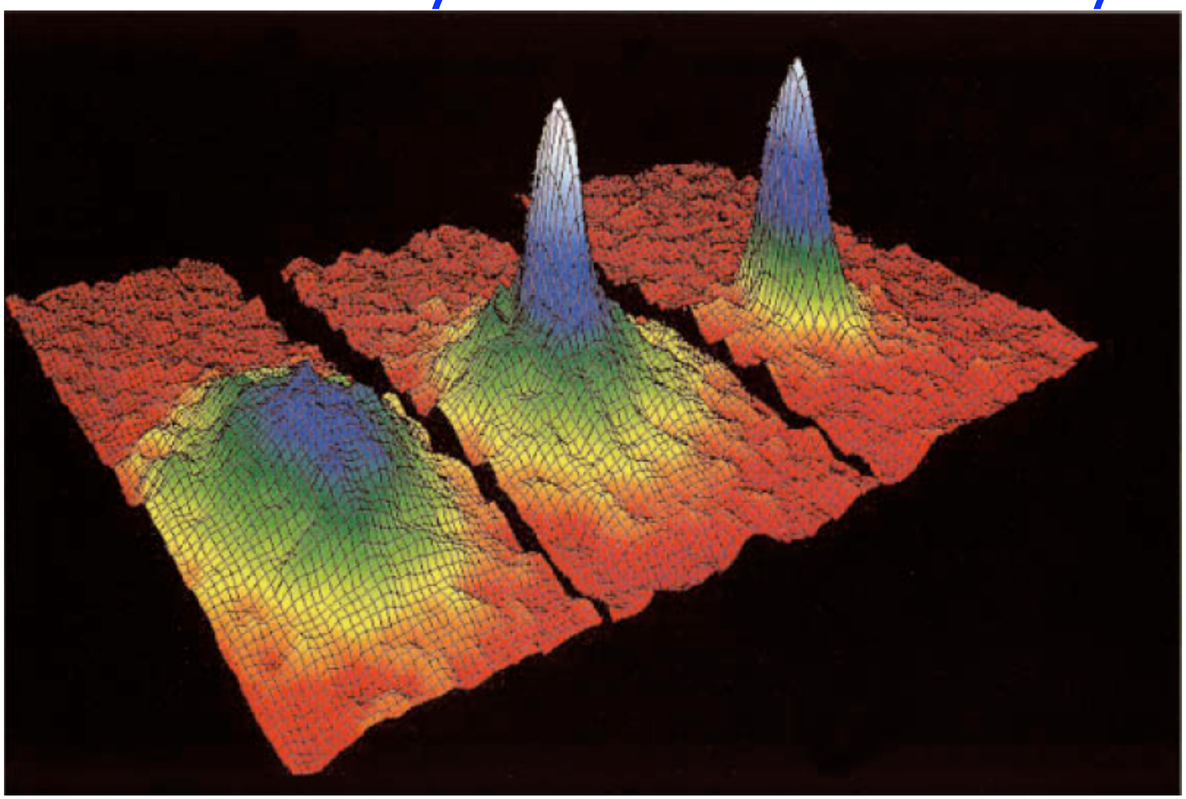
Eric A. Cornell	Wolfgang Ketterle	Carl E. Wieman
1/3 of the prize	1/3 of the prize	1/3 of the prize
USA	Federal Republic of Germany	USA
University of Colorado, JILA Boulder, CO, USA	Massachusetts Institute of Technology (MIT) Cambridge, MA, USA	University of Colorado, JILA Boulder, CO, USA
b. 1961	b. 1957	b. 1951

Oscillators

- Eigenvalues $\varepsilon_{n_x n_y n_z} = (n_x + \frac{1}{2})\,\hbar\omega_x + (n_y + \frac{1}{2})\,\hbar\omega_y + (n_z + \frac{1}{2})\,\hbar\omega_z$
- Ground state: all atoms in state with $n_x = n_y = n_z = 0$
- Wave function $\phi_{000}(\boldsymbol{r}) = \left(\frac{m\omega_{HO}}{\pi\hbar}\right)^{3/4} \exp\left\{-\frac{m}{2\hbar}(\omega_x x^2 + \omega_y y^2 + \omega_z z^2)\right\}$
- with $\omega_{HO} = (\omega_x \omega_y \omega_z)^{1/3}$
- N bosons in this sp state $|\Phi_0^N\rangle = \frac{1}{\sqrt{N!}}(a_{000}^\dagger)^N\,|0\rangle$
- Calculate density $\rho(\boldsymbol{r}) = N\,|\phi_{000}(\boldsymbol{r})|^2$ grows with N
- shape does not and is determined by trap potential: $a_{HO} = \left(\frac{\hbar}{m\omega_{HO}}\right)^{1/2}$
- Actual scale $a_{HO} \approx 1\ \mu\mathrm{m}$
- Finite temperature: atoms occupy excited states
- For $k_B T \gg \hbar\omega_{HO}$ use classical Boltzmann distribution
- spherical $\rho_{cl}(r) \propto \exp\left\{-\frac{V_{ext}(r)}{k_B T}\right\}$ (Landau&Lifshitz)
- If $V_{ext}(r) = \frac{1}{2}m\omega_{HO}^2 r^2$ width $R_T = a_{HO}\left(\frac{k_B T}{\hbar\omega_{HO}}\right)^{1/2}$

BEC observation

- BEC observed in the form of sharp peak in the center
- Wave function in momentum space also Gaussian: width $\propto a_{HO}^{-1}$
- So both in coordinate space and momentum space
- Infinite system all particles zero momentum but no signature in coordinate space
- Observe velocity distribution/ density distribution



Anderson et al.

Science **269**, 198 (1995)

Rubidium atoms (velocity)

left: just above condensation

middle: just after

right: further cooled

asymmetric trap

Trapped bosons at finite temperature

- Interaction between bosons important for the actual shapes
- Still useful considerations for noninteracting bosons
- Number of particles $N = \sum_{n_x n_y n_z} \frac{1}{\exp\{\beta(\varepsilon_{n_x n_y n_z} - \mu)\} - 1}$
- Energy $E = \sum_{n_x n_y n_z} \frac{\varepsilon_{n_x n_y n_z}}{\exp\{\beta(\varepsilon_{n_x n_y n_z} - \mu)\} - 1}$
- Usual thermodynamic limit not possible
- Still separate lowest state from the sum with N_0
- As for infinite system: can be of order N when $\mu \rightarrow \mu_c = \frac{3}{2}\hbar\bar{\omega}$
- with $\bar{\omega} = (\omega_x + \omega_y + \omega_z)/3$
- This limit is reached for a critical temperature $T = T_c$

Convert to integrals

- Rewrite particle number

$$N - N_0 = \sum_{n_x \neq 0, n_y \neq 0, n_z \neq 0} \frac{1}{\exp\{\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)\} - 1}$$

- do numerically or for $N \to \infty$

$$N - N_0 = \int_0^\infty dn_x dn_y dn_z \; \frac{1}{\exp\{\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)\} - 1}$$

- semiclassical description: excitation energies $\gg$ level spacing
- valid for large N and $k_B T \gg \hbar\omega_{HO}$
- Integrate: $N - N_0 = \zeta(3) \left(\frac{k_B T}{\hbar\omega_{HO}}\right)^3$ $\qquad \zeta(3) \approx 1.202$
- Imposing $N_0 \to 0$ at T_c
- yields $k_B T_c = \hbar\omega_{HO} \left(\frac{N}{\zeta(3)}\right)^{1/3} = 0.94\ \hbar\omega_{HO}\ N^{1/3}$
- or $\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^3$
- Evaluate energy similarly etc.
- Interaction important as are finite size corrections

Gross-Pitaevskii (GP) equation

- Dilute system: average interparticle spacing $\rho^{-1/3}$ large compared to magnitude of scattering length, or $\rho|a|^3 << 1$
- Previous discussion suggests that HB mean-field can be applied in dilute case: replace V (even if strong) with the pseudo potential
- HB potential then becomes $W_{HB}(\boldsymbol{r}) = g(N-1)|\phi_c(\boldsymbol{r})|^2 \approx gN|\phi_c(\boldsymbol{r})|^2$
- HB equation $\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r})\right]\phi_c(\boldsymbol{r}) + gN|\phi_c(\boldsymbol{r})|^2\phi_c(\boldsymbol{r}) = \mu\phi_c(\boldsymbol{r})$
- Looks like nonlinear Schrödinger equation and is referred to as the time-independent Gross-Pitaevskii equation
- Condensate orbital also minimizes (with $\int d\boldsymbol{r}|\phi_c(\boldsymbol{r})|^2 = 1$)

$$E_0^{GP}/N = \int d\boldsymbol{r}\left(\frac{\hbar^2}{2m}|\nabla\phi_c(\boldsymbol{r})|^2 + U(\boldsymbol{r})|\phi_c(\boldsymbol{r})|^2 + \frac{gN}{2}|\phi_c(\boldsymbol{r})|^4\right)$$

- Time-dependent GP equation

$$\left[-\frac{1}{2m}\nabla^2 + U(\boldsymbol{r};t)\right]\phi_c(\boldsymbol{r};t) + gN|\phi_c(\boldsymbol{r},\boldsymbol{t})|^2\phi_c(\boldsymbol{r};t) = i\hbar\frac{\partial}{\partial t}\phi_c(\boldsymbol{r};t)$$

- GP and GP(t) all that is needed to explain most data BEC

Confined bosons in harmonic traps

- Confining potential well approximated by HO
$$U(\boldsymbol{r}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$
- usually with cylindrical symmetry (cigar or pancake)
- Include interaction at the GP level
- Effect can be large even when the system is dilute
- Estimate: assume condensate wave function approximately HO ground state $\phi_{000}(\boldsymbol{r})$ (see Ch. 5)
- Central density of condensate $\rho(0) = N|\phi_c(0)|^2 \approx N\left(\frac{m\omega_{HO}}{\pi\hbar}\right)^{3/2} = \frac{N}{\pi^{3/2}a_{HO}^3}$
- Typical values: 10^3<N<10^6, |a|~10^{-9}m, a_{HO}~10^{-6}m so $10^{-6} < \rho|a|^3 < 10^{-3}$
- So very dilute
- Consider mean-field potential $W_{HB}(0) = gN|\phi_c(0)|^2 \approx N\frac{a}{a_{HO}^3}\frac{4\hbar^2}{m\sqrt{\pi}}$

BEC in traps at the GP level

- Compare with HO energy scale $\hbar\omega_{HO} = \frac{\hbar^2}{m a_{HO}^2}$
- Ratio proportional to $u = N\frac{a}{a_{HO}}$
- Measure of strength of interaction effects
- For quoted values $1 < |u| < 10^3$
- So expect large deviations of GP w.r.t. noninteracting profile
- Example u~125

  $a = 2.75$ nm and a_{HO}=1.76 μm
- Column density $\bar{\rho}(z) = \int dy \rho(0,y,z)$
- 8×10^4 ^{23}Na atoms
- Trap $\omega_x = \omega_y = 2050$ rad/s and $\omega_z = 170$ rad/s
- Reduction of 12 w.r.t. HO only